



# **STIC Search Report**

## **Biotech-Chem Library**

**STIC Database Tracking Number: 159211**

**TO: Fiona Powers**  
**Location: REM/4A31/5C18**  
**Art Unit: 1626**  
**\_\_\_\_\_, 2005**

**Case Serial Number: 09/927685**

**From: P. Sheppard**  
**Location: Remsen Building**  
**Phone: (571) 272-2529**

**sheppard@uspto.gov**

### **Search Notes**

=> d his ful

(FILE 'REGISTRY' ENTERED AT 17:41:32 ON 09 AUG 2005)

L10 STR  
L12 STR L10  
L14 50 SEA SSS SAM L10 OR L12  
L15 101313 SEA SSS FUL L10 OR L12  
L43 STR  
L44 319 SEA SUB=L15 SSS FUL L43

FILE 'HCAPLUS' ENTERED AT 18:10:37 ON 09 AUG 2005

L45 193 SEA ABB=ON PLU=ON L44  
L48 21 SEA ABB=ON PLU=ON L45 AND (INK OR DYE OR INFRARED)  
D STAT QUE  
D IBIB ABS HITSTR L48 1-21

FILE HCAPLUS

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 9 Aug 2005 VOL 143 ISS 7  
FILE LAST UPDATED: 8 Aug 2005 (20050808/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 AUG 2005 HIGHEST RN 859027-58-0  
DICTIONARY FILE UPDATES: 8 AUG 2005 HIGHEST RN 859027-58-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Powers 09\_927685- History

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 18:10:37 ON 09 AUG 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 9 Aug 2005 VOL 143 ISS 7

FILE LAST UPDATED: 8 Aug 2005 (20050808/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

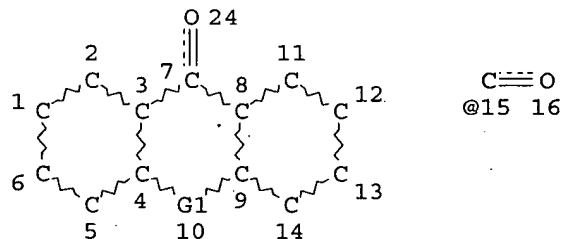
This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

=>

=> d stat que

L10 STR



VAR G1=15/O

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

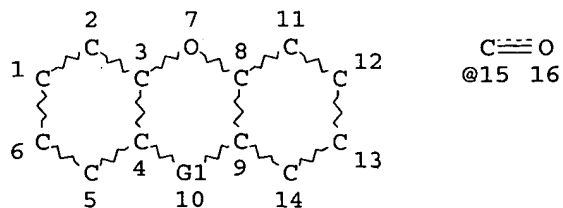
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

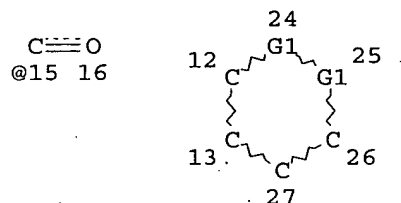
L12 STR



VAR G1=15/O  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE  
 L15 101313 SEA FILE=REGISTRY SSS FUL L10 OR L12  
 L43 STR



VAR G1=15/O  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE  
 L44 319 SEA FILE=REGISTRY SUB=L15 SSS FUL L43  
 L45 193 SEA FILE=HCAPLUS ABB=ON PLU=ON L44  
 L48 21 SEA FILE=HCAPLUS ABB=ON PLU=ON L45 AND (INK OR DYE OR INFRARED)

=>  
 =>

=> d ibib abs hitstr l48 1-21

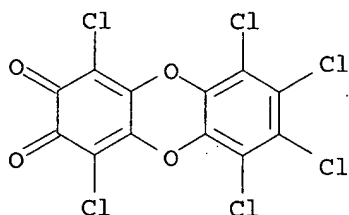
L48 ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2005:130455 HCAPLUS  
 DOCUMENT NUMBER: 142:373921  
 TITLE: Oxidative addition reaction of o-quinones to triphenylantimony: novel triphenylantimony catecholate complexes  
 AUTHOR(S): Cherkasov, Vladimir K.; Grunova, Ekaterina V.; Poddel'sky, Andrey I.; Fukin, Georgy K.; Kurskii, Yury A.; Abakumova, Ludmila G.; Abakumov, Gleb A.  
 CORPORATE SOURCE: G. A. Razuvaev Institute of Organometallic Chemistry, Laboratory of the Chemistry of Organoelemental Compounds, Russian Academy of Sciences, Nizhny Novgorod, 603950, Russia  
 SOURCE: Journal of Organometallic Chemistry (2005), 690(5), 1273-1281  
 CODEN: JORCAI; ISSN: 0022-328X  
 PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 142:373921

AB New catecholate Sb(V) complexes triphenyl(3,6-di-tert-butylcatecholato)antimony(V) Ph<sub>3</sub>Sb(3,6-DBCat) (1) and triphenyl(perchloroxanthrenecatecholato)antimony(V) Ph<sub>3</sub>Sb(OXCatCl) (2) were synthesized by the oxidative addition reaction of corresponding o-quinones (3,6-di-tert-butyl-o-benzoquinone and perchloroxanthrenequinone-2,3) with triphenylantimony. Catecholates 1 and 2 can alternatively be synthesized by reacting the appropriate thallium catecholate with triphenylantimony dichloride. The oxidative addition reaction of an equimolar ratio of 4,4'-di-(3-methyl-6-tert-butyl-o-benzoquinone) and triphenylantimony yielded 4-(2-methyl-5-tert-butyl-cyclohexadien-1,5-dion-3,4-yl)-(3-methyl-6-tert-butyl-catecholato)triphenylantimony(V) Ph<sub>3</sub>Sb(Cat-Q) (3); in the case of a 1:2 molar ratio, complex 4,4'-di-[(3-methyl-6-tert-butyl-catecholato)triphenylantimony(V)] Ph<sub>3</sub>Sb(Cat-Cat)SbPh<sub>3</sub> (4) resulted. Complexes 1-4 were characterized by IR and <sup>1</sup>H NMR spectroscopy. Mol. structures of 1, 2, and 4 were determined by X-ray crystallog. to be a distorted tetragonal-pyramidal.

IT 65005-72-3, Perchloroxanthrene-2,3-quinone  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation and structure of triphenylantimony catecholate complexes via oxidative addition of quinones to triphenylantimony)

RN 65005-72-3 HCAPLUS  
 CN Dibenzo[b,e][1,4]dioxin-2,3-dione, 1,4,6,7,8,9-hexachloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:132825 HCAPLUS

DOCUMENT NUMBER: 128:291941

TITLE: Comparison of reaction products from the transformation of catechol catalyzed by birnessite or tyrosinase

AUTHOR(S): Naidja, A.; Huang, P. M.; Bollag, J. -M.

CORPORATE SOURCE: Dep. of Soil Science, Univ. of Saskatchewan, Saskatoon, SK, S7N 5A8, Can.

SOURCE: Soil Science Society of America Journal (1998), 62(1), 188-195

CODEN: SSSJD4; ISSN: 0361-5995

PUBLISHER: Soil Science Society of America

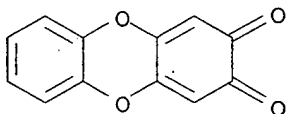
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Both tyrosinase, a Cu-containing polyphenoloxidase, and birnessite (δ-MnO<sub>2</sub>) are able to catalyze the transformation of phenolic compds. through oxidative polymerization, a process that leads to humification, but the reaction mechanisms are not fully understood. The objective of this study

was to characterize or identify the reaction products generated from catechol (1,2-dihydroxybenzene) by birnessite or tyrosinase. Birnessite and tyrosinase catalyzed the transformation of catechol to oligomers, polycondensates, and fragments. The reaction products formed after catalysis by tyrosinase were brown colored, while those resulting from the birnessite-catechol system were green colored; the former had a higher absorbance between 200 and 620 nm than the latter. This indicated a higher degree of aromatic ring condensation in products of the tyrosinase-catechol system relative to those of the birnessite-catechol system. In addition, the products of birnessite catalysis contained polycondensates and fragments, including aliphatic components, with lower mol. wts. than did the products derived from catalysis by tyrosinase. Fourier-transform IR (FTIR) anal. and mass spectrometry indicated that the reaction products formed an organic coating on the birnessite granules.

IT 6859-47-8, Diphenylenedioxide-2,3-quinone  
 RL: BSU (Biological study, unclassified); FMU (Formation, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)  
 (comparison of reaction products from transformation of catechol catalyzed by birnessite or tyrosinase)  
 RN 6859-47-8 HCAPLUS  
 CN Dibenzo[b,e][1,4]dioxin-2,3-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:192280 HCAPLUS

DOCUMENT NUMBER: 126:250248

TITLE: Supercritical extraction of the anthraquinone derivatives of the madder (*Rubia tinctorum*)

AUTHOR(S): Krizsan, Krisztina; Hollosy, Ferenc; Szokan, Gyula; Laszlo, Miklos

CORPORATE SOURCE: ELTE Szerves Kemiai Tanszek, Budapest, 1117, Hung.

SOURCE: Olaj, Szappan, Kozmetika (1996), 45(Spec. Issue), 66-69

CODEN: OSZKAT; ISSN: 0472-8602

PUBLISHER: METE

DOCUMENT TYPE: Journal

LANGUAGE: Hungarian

AB Expts. were performed to sep. some compds. (hydroxyanthraquinones, anthraquinone glycosides) from madder (*Rubia tinctorum*) cell suspension cultures. The aim was to find a sensitive and reproducible procedure to determine the composition of a sample from the bioreactor. Soxhlet extraction (MeOH),

supercrit. fluid extraction (CO<sub>2</sub>, MeOH) and solid-phase extraction (C18 silica) were

studied. A HPLC method was developed for the characterization of the sample. High extraction yield were obtained by supercrit. fluid extraction at 5,000

psi, using CO<sub>2</sub> + MeOH.

IT 50764-64-2P, Ruberitric acid

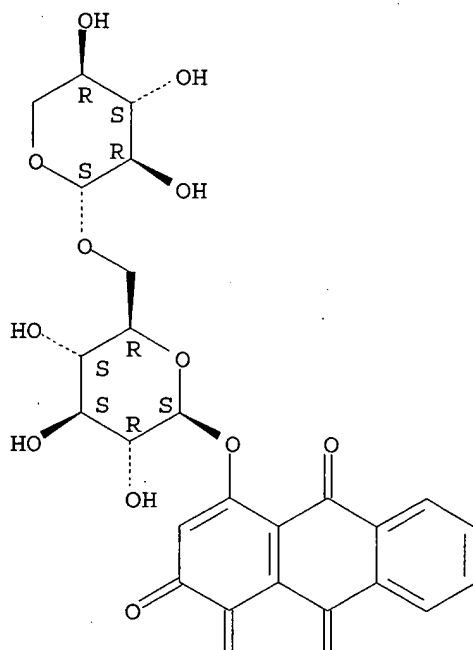
RL: PUR (Purification or recovery); PREP (Preparation)  
(supercrit. fluid extraction of anthraquinone derivs. from madder cell  
suspension culture)

RN 50764-64-2 HCAPLUS

CN 1,2,9,10-Anthracenetetrone, 4-[(6-O-β-D-xylopyranosyl-β-D-  
glucopyranosyl)oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



L48 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1995:908299 HCAPLUS  
DOCUMENT NUMBER: 124:248641  
TITLE: Synthesis and thermolysis reactions of molecular  
complexes of bis[tris(trifluoromethyl)germyl]mercury(I  
I) with o-quinones  
AUTHOR(S): Abakumov, G. A.; Cherkasov, V. K.; Ermolaev, N. I.;  
Nevodhikov, V. I.; Abakumova, L. G.  
CORPORATE SOURCE: Inst. Organometallic Chem., Russian Acad. Sci.,  
Nizhnii Novgorod, 603600, Russia  
SOURCE: Izvestiya Akademii Nauk, Seriya Khimicheskaya (1995),  
(8), 1568-73  
CODEN: IASKEA  
PUBLISHER: Nauka  
DOCUMENT TYPE: Journal



LANGUAGE: Russian

AB The stable mol. complexes of bis[tris(trifluoromethyl)germyl]mercury(II) [(CF<sub>3</sub>)<sub>3</sub>Ge]<sub>2</sub>Hg (1) with o-quinones (3,6-di-tert-butyl-1,2-benzoquinone (2), 3,6-di-tert-butyl-4,5-dimethoxy-1,2-benzoquinone (3), and 1,4,5,7-tetra-tert-butyl-9,10-dioxo-2,3-anthracenedione (4)) was synthesized and characterized by elemental anal., IR and electron absorption spectroscopy methods. Depending on the starting reagents ratio the complexes were prepared R<sub>2</sub>Hg·Q (5, 7, 9) and R<sub>2</sub>Hg·Q<sub>2</sub> (6, 8, 10), where Q = 2 (5, 6), 3 (7, 8), 4 (9, 10); R = Ge(CF<sub>3</sub>)<sub>3</sub>. According to the spectral data in the R<sub>2</sub>Hg·Q complexes mol. of o-quinone appears as the neutral ligand, whereas in the R<sub>2</sub>Hg·Q<sub>2</sub> complexes the 2nd mol. of o-quinone is associated noncoordinatively with 1. It was established by the ESR method that the thermolysis of polycryst. samples of 6 and 10 occurs with formation of the intermediate radical pairs that results in the paramagnetic o-semiquinone complexes SQGe(CF<sub>3</sub>)<sub>3</sub> - the typical products of the 1-electron oxidation of the organometallic compds. by o-quinones.

IT 173256-55-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 173256-55-8 HCAPLUS

CN Mercury, [1,4,6,8-tetrakis(1,1-dimethylethyl)dibenzo[b,e][1,4]dioxin-2,3-diolato(2-)-O<sub>2</sub>,O<sub>3</sub>]bis[tris(trifluoromethyl)germyl]-, (T-4)-, compd. with 1,4,6,8-tetrakis(1,1-dimethylethyl)dibenzo[b,e][1,4]dioxin-2,3-dione (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 172986-37-7

CMF C28 H38 O4

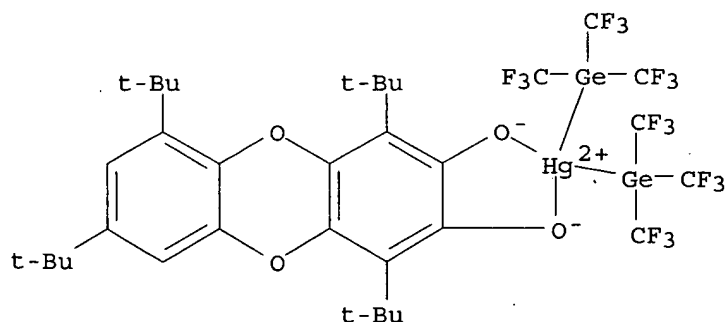
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

CM 2

CRN 172986-36-6

CMF C34 H38 F18 Ge2 Hg O4

CCI CCS



IT 172986-37-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with bis(tris(trifluoromethyl)germyl)mercury)

RN 172986-37-7 HCAPLUS

CN Dibenzo[b,e][1,4]dioxin-2,3-dione, 1,4,6,8-tetrakis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

L48 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:559446 HCAPLUS

DOCUMENT NUMBER: 119:159446

TITLE: Analysis of reaction kinetics by Fourier transform infrared spectrometry. Laser-induced photochemistry of 1,2-benzoquinones

AUTHOR(S): Alkenings, B.; Bettermann, H.; Dasting, I.; Schroers, H. J.

CORPORATE SOURCE: Inst. Phys. Chem. Elektrochem., Heinrich-Heine-Univ., Duesseldorf, W-4000, Germany

SOURCE: Vibrational Spectroscopy (1993), 5(1), 43-9  
CODEN: VISPEK; ISSN: 0924-2031

DOCUMENT TYPE: Journal

LANGUAGE: English

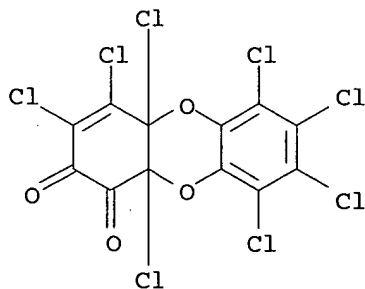
AB Photokinetic studies of an intermol. [4 + 2] photocycloaddn. starting from 3,4,5,6-tetrachloro-1,2-benzoquinone (o-chloranil) and of CO elimination from 3,5-di-tert-butyl-1,2-benzoquinone (DBQ) are reported. Both reactions were initiated by exciting the lowest energetic  $1(\pi-\pi)^*$  [and also the  $1(n-\pi)^*$  state in the case of DBQ] with argon ion laser emission lines. The kinetic analyze were mostly carried out with the use of time-dependent IR intensity alterations in the range of C=O stretching modes. The reactions have a non-uniform character which reveals the existence of intermediates. The intermediate of the dimerization could be established by the wavelength-dependent quantum yield related to the initial compound. The laser-induced reaction can be described by a two-photon process in which the first photon excites the starting compound while the second photon interacts with the intermediate. In the case of the CO elimination, the bis-ketene intermediate could be identified by recording the asym. stretching vibration at 2173  $\text{cm}^{-1}$  in the vicinity of the vibration of free carbon monoxide at 2134  $\text{cm}^{-1}$ .

IT 136672-44-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 136672-44-1 HCAPLUS

CN Dibenzo[b,e][1,4]dioxin-1,2-dione, 3,4,4a,6,7,8,9,10a-octachloro-4a,10a-dihydro- (9CI) (CA INDEX NAME)



L48 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:593901 HCAPLUS

DOCUMENT NUMBER: 115:193901

TITLE: Laser-induced intermolecular photocycloaddition of 3,4,5,6-tetrachloro-1,2-benzoquinone

AUTHOR(S): Bettermann, H.; Schroers, H. J.

CORPORATE SOURCE: Inst. Phys. Chem., Heinrich-Heine-Univ., Duesseldorf,

SOURCE: D-4000, Germany  
Spectrochimica Acta, Part A: Molecular and  
Biomolecular Spectroscopy (1991), 47A(7), 893-6  
CODEN: SAMCAS; ISSN: 0584-8539

DOCUMENT TYPE: Journal

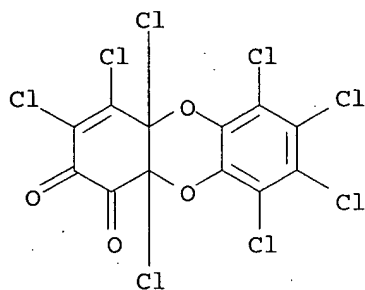
LANGUAGE: English

AB An intermol. [4+2] photocycloaddn. was initiated by excitation of the lowest energetic  $1(\pi-\pi^*)$  state of o-chloranil (3,4,5,6-tetrachloro-1,2-benzoquinone) using emission lines of an argon ion laser. The course of reaction was investigated by measuring the IR spectra of the reaction mixture. The reaction has non-uniform character and shows a wavelength-dependence of the quantum yield. For these reasons, this laser-induced reaction is described by a two-photon process in which the first photon excites the initial compound and the second photon interacts with an intermediate generating the final compound

IT 136672-44-1P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in laser-induced two-photon intermol. photocycloaddn. of tetrachlorobenzoquinone)

RN 136672-44-1 HCAPLUS

CN Dibenzo[b,e][1,4]dioxin-1,2-dione, 3,4,4a,6,7,8,9,10a-octachloro-4a,10a-dihydro- (9CI) (CA INDEX NAME)



L48 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:641439 HCAPLUS

DOCUMENT NUMBER: 113:241439

TITLE: Electrophotographic photoreceptors containing azo dyes

INVENTOR(S): Kanamaru, Tetsuo

PATENT ASSIGNEE(S): Canon K. K., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.  
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02054275	A2	19900223	JP 1988-204736	19880819
PRIORITY APPLN. INFO.:			JP 1988-204736	19880819
OTHER SOURCE(S):	MARPAT 113:241439			

AB Electrophotog. photoreceptors, characterized by high sensitivity and stability of elec. potential during repeated usage, consist of 2 photosensitive layers on an elec. conductive support, i.e. a charge-transporting layer and a charge-generating layer containing an azo

**dye** Cp1N:NAr1[C(:Z)NH]mW[C(:Z)NH]nAr2N:NCp1 [I; W = single bond, divalent aromatic hydrocarbon, or heterocycle; Ar1,Ar2 = (un)substituted divalent cyclic ketone or cyclic quinone; Cp1,Cp2 = coupler containing phenolic OH; Z = O, S; m,n = 0 or 1; and m = n ≠ 0]. Photoreceptors containing I in a charge-generating layer showed surface potential of -675 to -720 V and E1/2 (amount of light exposure necessary to attenuate 1/2 the elec. potential reached after 1 s attenuation in the dark) of 2.5-3.3 lx-s.

IT 129781-92-6P

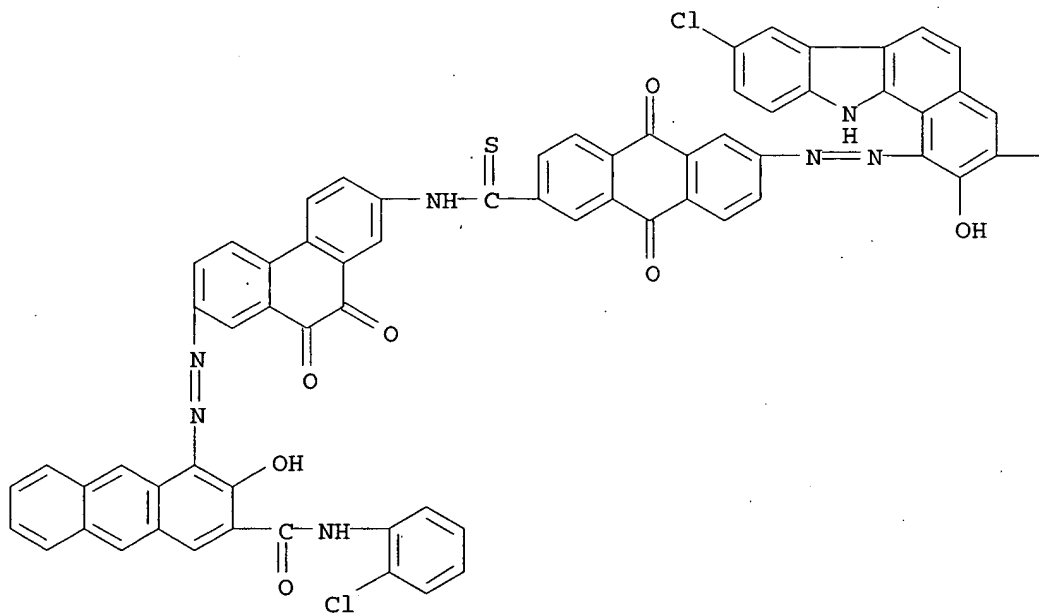
RL: PREP (Preparation)

(preparation of, for electrophotog. photoconductor)

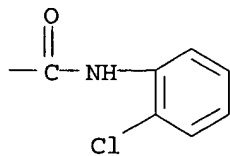
RN 129781-92-6 HCAPLUS

CN 11H-Benzo[a]carbazole-3-carboxamide, 8-chloro-N-(2-chlorophenyl)-1-[[6-[[[7-[[3-[[[(2-chlorophenyl)amino]carbonyl]-2-hydroxy-1-anthracenyl]azo]-9,10-dihydro-9,10-dioxo-2-phenanthrenyl]amino]thioxomethyl]-9,10-dihydro-9,10-dioxo-2-anthracenyl]azo]-2-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



ACCESSION NUMBER: 1987:51699 HCAPLUS  
 DOCUMENT NUMBER: 106:51699  
 TITLE: Pigments for polarizing films  
 INVENTOR(S): Nakamura, Katsuji; Fujio, Junichi; Hosonuma, Makoto;  
 Nakatsuka, Masakatsu; Nishizawa, Isao  
 PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61087757	A2	19860506	JP 1984-210067	19841005
JP 04030986	B4	19920525		
DE 3590479	T	19861030	DE 1985-3590479	19850612
DE 3590479	C2	19921224		
EP 198082	B1	19920715	EP 1985-903035	19850612
R: FR, IT				
US 4824882	A	19890425	US 1986-866492	19860520
US 5059356	A	19911022	US 1990-579246	19900906
US 5286418	A	19940215	US 1991-725641	19910703
US 5354513	A	19941011	US 1993-135420	19931013
PRIORITY APPLN. INFO.:			JP 1984-210067	A 19841005
			WO 1985-JP328	W 19850612
			US 1986-866492	A3 19860520
			US 1989-308031	B1 19890227
			US 1990-579246	A3 19900906
			US 1991-725641	A3 19910703

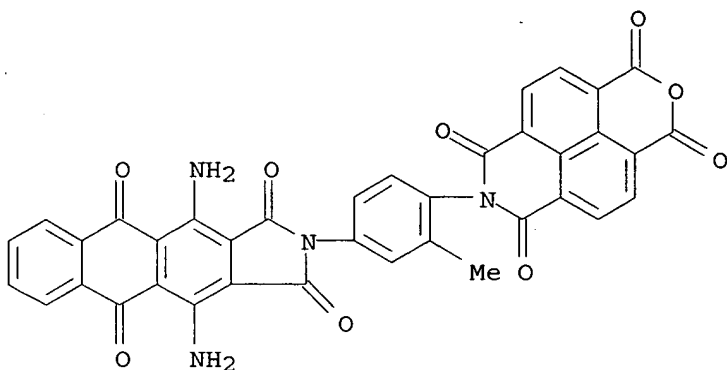
GI For diagram(s), see printed CA Issue.

AB Polarizer film pigments I [n = 1, 2; R-R5 = H, halo, OH, NH2, C1-3 alkylamino ( $\geq 1$  of R, R3-R5 is OH or amino); R6, R7 = H, halo, Me; R8 = CO2H, CO2R9, CONH2, CONHR9, O2CR9, NHCOR9, N:NR9, Q; A = substituted benzene, naphthalene, anthraquinone nucleus; R9 = (un)substituted Ph; X = O, S, NH] **dye** polymer films for use as polarizers. Thus, 1,4-diaminoanthraquinone-2,3-dicarboxylic anhydride was refluxed with BzNHC6H4NH2-4 in DMF for 5 h, forming I (n = 1, R = R1 = R2 = R3 = R6 = R7 = H, R4 = R5 = NH2, R8 = NHBz, X = O),  $\lambda_{\max}$  680 nm (PhNO2). Poly(ethylene terephthalate) pellets were dyed with 0.2% I, made into a film, drawn, and set to form a 70- $\mu$ -thick polarizer film with  $\lambda_{\max}$  685 nm and a polarization degree of 88% (685 nm), which showed no change in color or decline in polarization degree after 500 h exposure to 90% relative humidity at 80°.

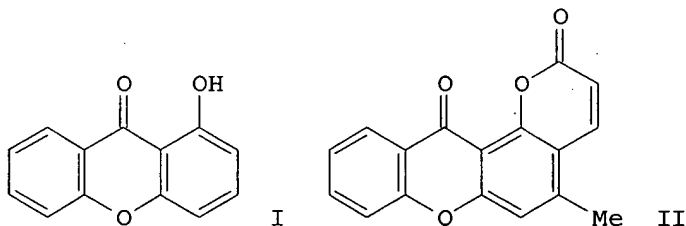
IT **106307-97-5P**  
 RL: PREP (Preparation)  
 (manufacture of, as polarizing **dye** for plastic films)

RN 106307-97-5 HCAPLUS

CN 1H-2-Benzopyrano[6,5,4-def]isoquinoline-1,3,6,8(7H)-tetrone,  
 7-[4-(4,11-diamino-1,3,5,10-tetrahydro-1,3,5,10-tetraoxo-2H-naphth[2,3-f]isoindol-2-yl)-2-methylphenyl]- (9CI) (CA INDEX NAME)



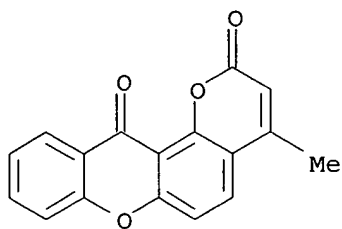
L48 ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1983:575540 HCAPLUS  
 DOCUMENT NUMBER: 99:175540  
 TITLE: Studies in synthesis of xanthone derivatives: Part III. A new one-step synthesis of xanthenes  
 AUTHOR(S): Patolia, Ravji J.; Trivedi, K. N.  
 CORPORATE SOURCE: Fac. Sci., M. S. Univ. Baroda, Baroda, 390 002, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(5), 444-7  
 CODEN: IJSBDB; ISSN: 0376-4699  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 99:175540  
 GI



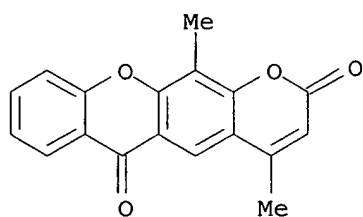
AB Et salicylate condenses with different phenols in refluxing Ph2O to give various xanthenes, e.g., I, in good yields. With resorcinol, hydroquinone, catechol, and 3,4-xylenol, the corresponding Ph salicylate derivs. are also obtained. Condensation with hydroxycoumarins gives pyranoxanthenes, e.g., II, which can not be prepared by the Pechmann condensation of hydroxyxanthenes. The structures of the intermediates and final products are established by spectral data (IR, H and <sup>13</sup>C NMR).

IT 87504-05-0P 87504-06-1P 87504-07-2P  
 87504-08-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

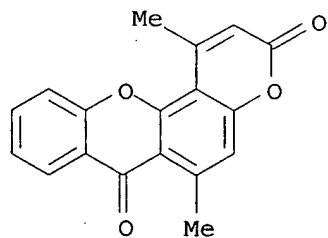
RN 87504-05-0 HCAPLUS  
 CN 2H,12H-Pyrano[2,3-a]xanthene-2,12-dione, 4-methyl- (9CI) (CA INDEX NAME)



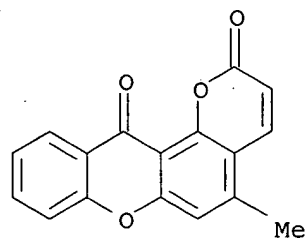
RN 87504-06-1 HCAPLUS  
CN 2H,6H-Pyrano[3,2-b]xanthene-2,6-dione, 4,12-dimethyl- (9CI) (CA INDEX NAME)



RN 87504-07-2 HCAPLUS  
CN 3H,7H-Pyrano[2,3-c]xanthene-3,7-dione, 1,6-dimethyl- (9CI) (CA INDEX NAME)

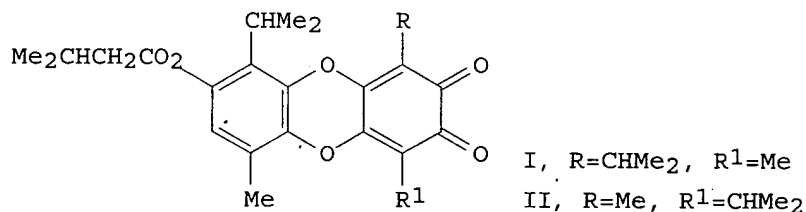


RN 87504-08-3 HCAPLUS  
CN 2H,12H-Pyrano[2,3-a]xanthene-2,12-dione, 5-methyl- (9CI) (CA INDEX NAME)

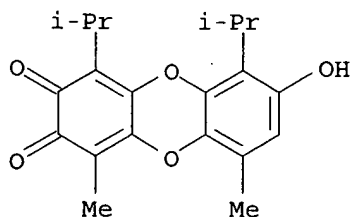


L48 ANSWER 10 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1980:160548 HCAPLUS

DOCUMENT NUMBER: 92:160548  
 TITLE: Leaf-gland pigments from Labiatae: ecklonoquinones A and B, two novel dibenzo-p-dioxine-o-quinones from *Plectranthus ecklonii* Benth  
 AUTHOR(S): Uchida, Masaaki; Ruedi, Peter; Eugster, Conrad Hans  
 CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich-Irchel, Zurich, CH-8057, Switz.  
 SOURCE: Helvetica Chimica Acta (1980), 63(1), 225-31  
 CODEN: HCACAV; ISSN: 0018-019X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 GI

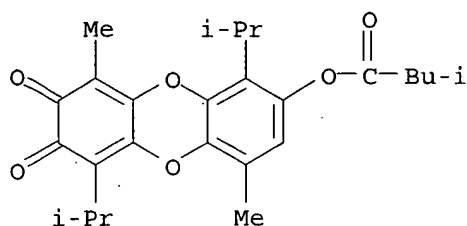


AB The novel isomeric dibenzo-p-dioxine o-quinones ecklonoquinone A (I) and ecklonoquinone B(II) were isolated from leaves of *P. ecklonii*, in addition to 2(S)-5,4'-dihydroxy-6,7-dimethoxyflavanone, cirsimaritin, and parvifloron F. UV, IR, mass, and extensive 1H- and 13C-NMR data are given for I and II.  
 IT 73328-58-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 73328-58-2 HCAPLUS  
 CN Dibenzo[b,e][1,4]dioxin-2,3-dione, 7-hydroxy-1,9-dimethyl-4,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



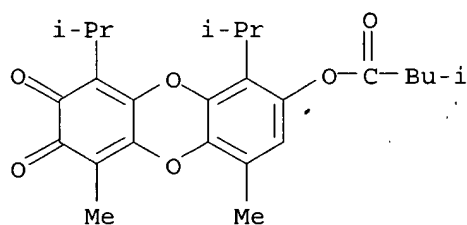
IT 73328-28-6 73328-29-7  
 RL: BIOL (Biological study) (Plectranthus dibenzodioxine orthoquinone, structure of)  
 RN 73328-28-6 HCAPLUS  
 CN Butanoic acid, 3-methyl-, 7,8-dihydro-4,9-dimethyl-1,6-bis(1-methylethyl)-7,8-dioxodibenzo[b,e][1,4]dioxin-2-yl ester (9CI) (CA INDEX NAME)





RN 73328-29-7 HCAPLUS

CN Butanoic acid, 3-methyl-, 7,8-dihydro-4,6-dimethyl-1,9-bis(1-methylethyl)-7,8-dioxodibenzo[b,e][1,4]dioxin-2-yl ester (9CI) (CA INDEX NAME)



L48 ANSWER 11 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:402933 HCAPLUS

DOCUMENT NUMBER: 67:2933

TITLE: Addition of arenesulfinic acids to 1,2,9,10-anthradiquinones

AUTHOR(S): Gorelik, M. V.

CORPORATE SOURCE: Res. Inst. Org. Intermeds. Dyes, Moscow, USSR

SOURCE: Zhurnal Vsesoyuznogo Khimicheskogo Obshchestva im. D. I. Mendeleeva (1966), 11(5), 586-7

CODEN: ZVKOA6; ISSN: 0373-0247

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB 1,2,9,10-Anthradiquinone and PhSO<sub>2</sub>H in EtOH or AcOH gave 80% mixed 4- and 3-phenylsulfonyl-1,2-dihydroxyanthraquinones, m. 273.5-4.5°, and m. 246-7°, resp. in nearly 1:1 ratio. Only the latter isomer formed from such addition of PhSO<sub>2</sub>Na in EtOH or dioxane. The sulfones were separated as

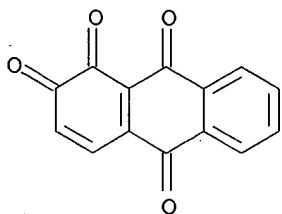
Me ethers formed with Me<sub>2</sub>SO<sub>4</sub>-K<sub>2</sub>CO<sub>3</sub> in Me<sub>2</sub>CO, when the 4-isomer yields the dimethoxy derivative in an interval that converts the 3-isomer (I) only to the 2-methoxy derivative, m. 216-17°; 1,2-dimethoxy derivative m. 171-1.5°. 3-Bromoalizarin and PhSO<sub>2</sub>Na in (CH<sub>2</sub>OH)<sub>2</sub> gave I. 3-Bromo-1,2,9,10-anthradiquinone and PhSO<sub>2</sub>H gave 48% 3-phenylsulfonylalizarin O1-benzenesulfonate, m. 196-7°; its 2-methoxy analog m. 231-2°. Ir spectra were reported.

IT 5539-67-3D, 1,2,9,10-Anthracenetetrone, derivs.

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactions with arenesulfinic acids)

RN 5539-67-3 HCAPLUS

CN 1,2,9,10-Anthracenetetrone (7CI, 8CI, 9CI) (CA INDEX NAME)



L48 ANSWER 12 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:55337 HCAPLUS

DOCUMENT NUMBER: 66:55337

TITLE: Furano compounds. VIII. Synthesis and infrared spectra of some furano- and pyranoxanthenes

AUTHOR(S): Puranik, Gurubasav S.; Rajagopal, Srinivasa

CORPORATE SOURCE: Univ. Karnatak, Dharwar, India

SOURCE: Indian Journal of Chemistry (1966), 4(10), 442-4

CODEN: IJOCAP; ISSN: 0019-5103

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. CA 65, 12185e. 3-Hydroxy-6-methylxanthone (4.52 g.) (CA 60, 15847e), 18 g. hexamine, and 565 ml. HOAc was heated 7 hrs. on a steam bath. The reaction mixture was cooled, and concentrated in vacuo to 200 ml., 9 ml. 1:1

HCl

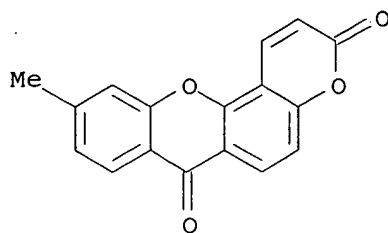
added, and the mixture refluxed 10 min., poured into H<sub>2</sub>O, and left overnight to yield 1.62 g. 4-formyl-3-hydroxy-6-methylxanthone (I), m. 218° (EtOH) (scarlet-red ferric reaction) (2,4-dinitrophenylhydrazones, m. >300° (HOAc)). I on heating 2 hrs. with Ac<sub>2</sub>O and few drops C<sub>5</sub>H<sub>5</sub>N yielded the 3-acetoxy compound, m. 150° (EtOH). I (0.42 g.), 0.52 g. BrCH(CO<sub>2</sub>Et)<sub>2</sub>, and 2 g. anhydrous K<sub>2</sub>CO<sub>3</sub> was refluxed 8 hrs. to yield 0.22 g. 5'-carbethoxyfurano[3',2':4,3]-6-methylxanthone (IIa) (R = Me, R<sub>1</sub> = H, R<sub>2</sub> = CO<sub>2</sub>Et) (II), m. 199° (EtOH). II (0.15 g.) in 20 ml. Me<sub>2</sub>CO was treated with 10 ml. 5% Na<sub>2</sub>CO<sub>3</sub>, the mixture refluxed 3 hrs., and acidified with 10 ml. dilute HCl, and the Me<sub>2</sub>CO distilled to yield 0.09 g. 5'-carboxyfurano[3',2':4,3]-6-methylxanthone (III), m. 315° (HOAc). Decarboxylation of 0.06 g. III by heating 20 min. at 190-200° with 0.06 g. Cu powder in 2 ml. quinoline in N atmospheric yielded 0.03 g. furano[3',2':4,3]-6-methylxanthone (IV), m. 207° (EtOH). A mixture of 0.12 g. I, 0.05 g. freshly fused NaOAc and 2 ml. Ac<sub>2</sub>O was heated 2 hrs. at 120° and then stirred 5 hrs. at 180° to yield 6'-pyrono[3',2':4,3]-6-methylxanthone (V), m. 257° (HOAc). The ir spectra of IV, V, and the following xanthenes were recorded and interpreted: 5'-methylfurano[3',-2':4,3]xanthone, furano[3',2':4,3]xanthone, 6'-pyrono[3',2':4,3]xanthone, 4'-methylfurano[3',2':4,3]xanthone, 5',6'-dimethylfurano[3',2':4,3]xanthenes, and 4',6'-dimethylfurano[3',2':4,3]xanthenes.

IT 14727-16-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 14727-16-3 HCAPLUS

CN 3H,7H-Pyrano[2,3-c]xanthene-3,7-dione, 10-methyl- (8CI) (CA INDEX NAME)

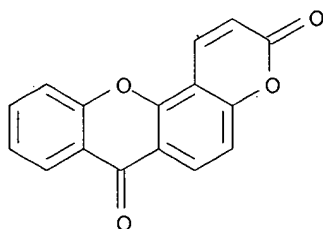


IT 6048-45-9

RL: PRP (Properties)  
(spectrum (ir) of)

RN 6048-45-9 HCAPLUS

CN 3H,7H-Pyrano[2,3-c]xanthene-3,7-dione (8CI, 9CI) (CA INDEX NAME)



L48 ANSWER 13 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1965:481165 HCAPLUS

DOCUMENT NUMBER: 63:81165

ORIGINAL REFERENCE NO.: 63:15024g-h,15025a-b

TITLE: 2,5-Bis(2-anthraquinonyl)-1,3,4-oxadiazole  
dyes

PATENT ASSIGNEE(S): CIBA Ltd.

SOURCE: 25 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 650257		19650108	BE	
FR 1404010			FR	
GB 1006157			GB	

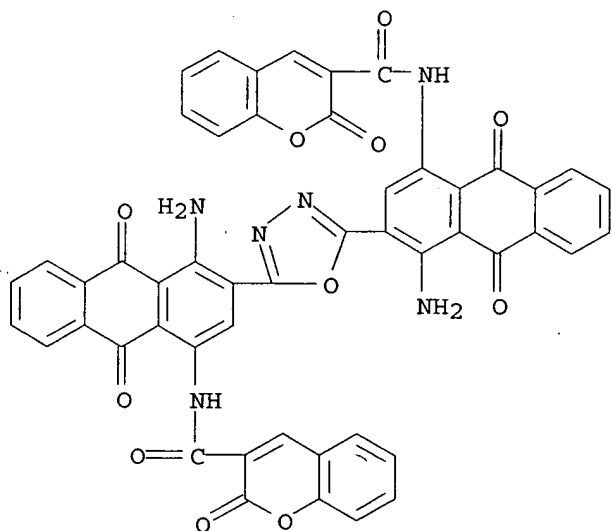
PRIORITY APPLN. INFO.: CH 19630709

GI For diagram(s), see printed CA Issue.

AB Comps. of the general formulas I and II give fast blue dyeings on cellulose fibers (III). Thus, a mixture of 2.8 parts thiophene-2-carboxylic acid, 150 parts PhNO<sub>2</sub>, and 7.1 parts SOCl<sub>2</sub> is agitated 1 hr. at 100-10°, the excess SOCl<sub>2</sub> and PhNO<sub>2</sub> are distilled, 5.4 parts 2,5-bis(1,4-diamino-2-anthraquinonyl)-1,3,4-oxadiazole is added at 100° and the mixture is heated 2 hrs. at 140-5°, heated 3 hrs. at 160-5°, and filtered at 120° to give I (Ar = 2-thienyl), blue on III. Similarly prepared are the following I (Ar and color on III given): 2-furyl, reddish blue; 2-quinolyl, reddish blue; 2-pyridyl, reddish blue; 1-phenyl, 1,2,3-triazol-4-yl, reddish blue; 5-phenyl-2-thienyl, greenish blue; 2-phenyl-5-thiazolyl, blue;

2-phenyl-4-quinolyl, blue; 3-coumarinyl, greenish blue; 2-benzofuranyl, blue; 2,4,6-trichloro-3-pyridyl, violet; 5-(2-furyl)-2-thienyl, greenish blue; 5-(5-phenyl-1,3,4-oxadiazol-2-yl)-2-thienyl, greenish blue; A, blue. Also prepared are the following II (Ar, Ar', and color on III given): Ph, 2-furyl, blue; Ph, 5-carbomethoxy-2-thienyl, greenish blue; 2-furyl, 5-carboxy-2-thienyl (Na salt), greenish blue.

IT 4375-75-1, Coumarin, 3,3'-[1,3,4-oxadiazole-2,5-diylbis[(4-amino-3,1-anthraquinonylene)iminocarbonyl]]di-  
(preparation of)  
RN 4375-75-1 HCAPLUS  
CN Coumarin, 3,3'-[1,3,4-oxadiazole-2,5-diylbis[(4-amino-3,1-anthraquinonylene)iminocarbonyl]]di- (7CI, 8CI) (CA INDEX NAME)



L48 ANSWER 14 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1961:76047 HCAPLUS

DOCUMENT NUMBER: 55:76047

ORIGINAL REFERENCE NO.: 55:14408b-d

TITLE: Anthraquinone and anthrone series. XXV. Constitution of nitrated dibenzanthrone

AUTHOR(S): Malhotra, S. S.; Unni, M. K.; Venkataraman, K.

CORPORATE SOURCE: Natl. Chem. Lab., Poona

SOURCE: Journal of Scientific & Industrial Research (1960), 19B, 382-90

CODEN: JSIRAC; ISSN: 0022-4456

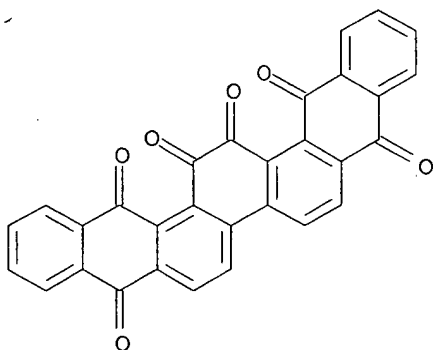
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 55, 8864i. The essential constituent of com. nitrated dibenzanthrone was shown to be 16-nitrodibenzanthrone (I), isolated from Caledon Black BB and Cibane Black BB by chromatography on alumina at 110°, also prepared by nitration of dibenzanthrone (II). I with H<sub>2</sub>CrO<sub>4</sub> and H<sub>2</sub>SO<sub>4</sub> gave 70% 1,2,7,8-diphthaloylphenanthraquinone (III), brown needles (C<sub>26</sub>H<sub>16</sub>O<sub>8</sub>), but further oxidation yielded 65% 2,2'-dianthraquinonyl-1,1'-dicarboxylic acid, m. 360° (decomposition). Decarboxylation with Cu in boiling quinoline gave 2,2'-bianthraquinonyl, yellow needles, m. 395-7°. This showed the nitro group was at position 15 or 16. The 16 position was confirmed by reduction of the isolated nitrodibenzanthrone to 16-aminodibenzanthrone (IV), also prepared from

benzanthrone and 2-aminobenzanthrone (V). 16,17-Diaminodibenzanthrone (VI) was also prepared by bimol. fusion of V. III was further obtained by oxidation of 16,17-dimeth oxydibenzanthrone (VII). **Infrared** data were given for I, II, IV, VI, VII, and 16-benzamidodibenzanthrone.

IT 121655-82-1, Dibenzo[b,n]picene-5,10,15,16,17,18-hexone  
(preparation of)  
RN 121655-82-1 HCAPLUS  
CN Dibenzo[b,n]picene-5,10,15,16,17,18-hexone (6CI) (CA INDEX NAME)



L48 ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1958:21014 HCAPLUS

DOCUMENT NUMBER: 52:21014

ORIGINAL REFERENCE NO.: 52:3754b-e

TITLE: Synthesis of 5-benzoylacenaphthene,  
5-(o-carboxybenzoyl)acenaphthene and its  
derivatives

AUTHOR(S): Akiyoshi, Saburo; Tsuge, Otohiko

CORPORATE SOURCE: Kyushu Univ., Fukuoka

SOURCE: Kogyo Kagaku Zasshi (1956), 59, 455-8

CODEN: KGKZA7; ISSN: 0368-5462

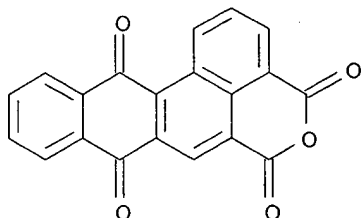
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The mixed m.p. curve for 5-benzoylacenaphthene (I), obtained by Friedel-Crafts reaction from acenaphthene (II) and benzoyl chloride in  $\text{PhNO}_2$ , and II is given, the azeotropic point being  $65^\circ$  (41.95% II). The 5,6-phthaloyl derivative of II (III) was obtained in 61.8% yield from the 5-(o-carboxybenzoyl) derivative (IV) by melting with  $\text{AlCl}_3$ . 4,5-Phthaloylnaphthalic acid (V), m.  $345-7^\circ$ , was obtained from a reaction of III with  $\text{Na}_2\text{Cr}_2\text{O}_7$  after boiling for 3 hrs. in glacial  $\text{AcOH}$ . The anhydride of V (VI), needles, m.  $356-7^\circ$ , was obtained from V by boiling with concentrated  $\text{HNO}_3$ . Oxidation of IV with  $\text{Na}_2\text{Cr}_2\text{O}_7$  in glacial  $\text{AcOH}$  gave 4-(o-carboxybenzoyl)naphthalic acid, m.  $230-2^\circ$ , which further gave its acid anhydride (VII), crystals, m.  $240-240.5^\circ$  ( $\text{AcOH}$ ). Heating VII in concentrated  $\text{H}_2\text{SO}_4$  at  $190-5^\circ$  for 2.5 hrs. gave 3,4-phthaloylnaphthalic acid and its acid anhydride (VIII), m.  $315^\circ$ . VI and VIII were treated with various amines to give the corresponding amides. The m.ps. and some colors (vat dye) of newly found amides are given in the following. Derivs. of VI:  $\text{PhNH}_2$   $352-3^\circ$ ; p-phenetidine  $284-5.5^\circ$ ; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>  $346-7^\circ$ ; o-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>  $357-8.5^\circ$ ;  $\alpha$ -aminoanthraquinone  $378-9^\circ$ , brown;  $\beta$ -aminoanthraquinone  $360-2^\circ$ , orange-brown; and of VIII:  $\text{PhNH}_2$   $319-20^\circ$ ;  $\alpha$ -aminoanthraquinone  $331-3^\circ$ , dark brown;  $\beta$ -aminoanthraquinone  $315-18^\circ$ , dark

brown.

IT 22245-71-2, Benz[a]anthracene-4,5-dicarboxylic anhydride,  
7,12-dihydro-7,12-dioxo-  
(preparation of)  
RN 22245-71-2 HCAPLUS  
CN 4H,6H-Anthra[3,2,1-de][2]benzopyran-4,6,8,13-tetrone (9CI) (CA INDEX  
NAME).



L48 ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1953:60331 HCAPLUS

DOCUMENT NUMBER: 47:60331

ORIGINAL REFERENCE NO.: 47:10231b-e

TITLE: Studies in vat dyes. II.

Phenanthraquinonyl(anthraquinonyl)amines and their  
dyeing properties

AUTHOR(S): Desai, R. D.; Kumta, N. S.

CORPORATE SOURCE: Dept. of Chem. Technol., Bombay

SOURCE: Journal of Scientific & Industrial Research (1952),  
11B, 284-6

CODEN: JSIRAC; ISSN: 0022-4456

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

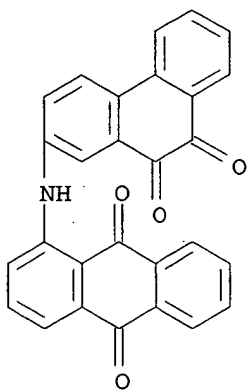
AB Vat dyes are prepared by condensing 2-bromophenanthraquinone (VI) and 3,6-dibromophenanthraquinone (VII) (Schmidt and Eitel, C.A. 26, 4337) with 1-amino- (VIII) or 2-amino- (IX) or 1-amino-2-methyl- (X) or 1,5-diaminoanthraquinone (XI) by the Ullman method. 1-(2-phenanthraquinonylamino)anthraquinone, m. >300° (red violet needles from EtOH-PhNO<sub>2</sub>), is prepared in 65% yield by refluxing VI, m. 233-4° (cf. Schmidt and Junghaus, Ber. 37, 3578(1904)), VIII, Cu<sub>2</sub>Cl<sub>2</sub>, and NaOAc in PhNO<sub>2</sub>. Similarly prepared (yield in parentheses) are 2-(2-phenanthraquinonylamino)anthraquinone (65%), m. >300° (brown plates from EtOH-pyridine), from VI and IX; 1-(2-phenanthraquinonylamino)-2-methylantraquinone (60%), m. >300° (violet plates from PhNO<sub>2</sub>), from VI and X; 1,5-bis(2-phenanthraquinonylamino)anthraquinone (65%), m. >300° (violet needles from PhNO<sub>2</sub>), from VI and XI; 3,6-bis(1-anthraquinonylamino)phenanthraquinone (65%), m. >340° (red brown needles from PhNO<sub>2</sub>), from VII and VIII; 3,6-bis(2-anthraquinonylamino)phenanthraquinone (65%), m. >340° (brown plates from EtOH-PhNO<sub>2</sub>), from VII and IX; 3,6-bis(2-methyl-1-anthraquinonylamino)phenanthraquinone (60%), m. >340° (violet plates from EtOH-PhNO<sub>2</sub>), from VII and X; and 3,6-bis(5-amino-1-anthraquinonylamino)phenanthraquinone (65%), m. >350° (red violet plates from PhNO<sub>2</sub>), from VII and XI. The dyes are soluble in concentrate H<sub>2</sub>SO<sub>4</sub> and give brown vats with alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>. All dyeings show excellent fastness to light and soaping, and moderate fastness to bleaching.

IT 75534-82-6, Phenanthrenequinone, 2-[1-anthraquinonylamino]-  
835917-61-8, Phenanthrenequinone, 3,6-bis[1-anthraquinonylamino]-  
855951-06-3, Anthraquinone, 1,1'-(9,10-dihydro-9,10-dioxo-3,6-

phenanthrylenediimino)bis[5-amino- 855951-13-2, Anthraquinone,  
1,1'-(9,10-dihydro-9,10-dioxo-3,6-phenanthrylenediimino)bis[2-methyl-  
(preparation of)

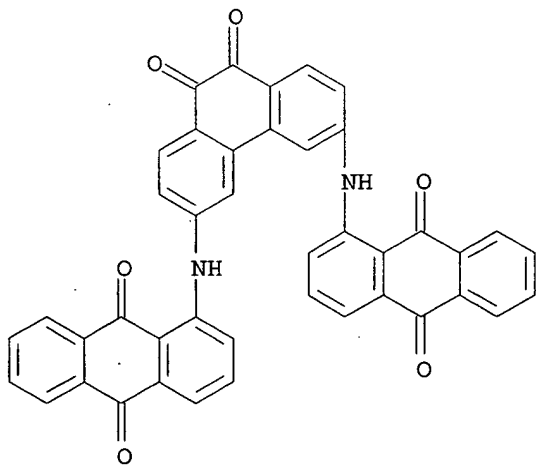
RN 75534-82-6 HCAPLUS

CN 9,10-Anthracenedione, 1-[(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)amino]-  
(9CI) (CA INDEX NAME)



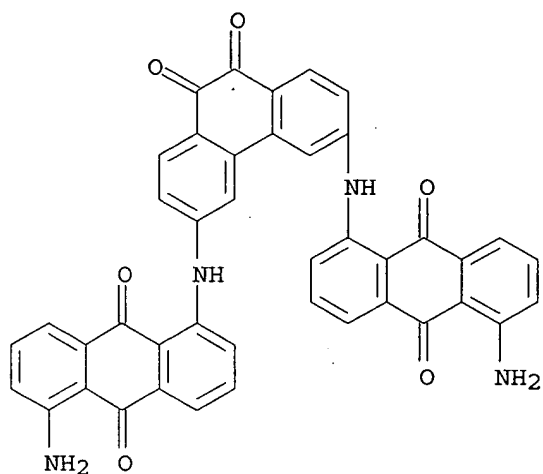
RN 835917-61-8 HCAPLUS

CN Phenanthrenequinone, 3,6-bis[1-anthraquinonylamino]- (5CI) (CA INDEX  
NAME)

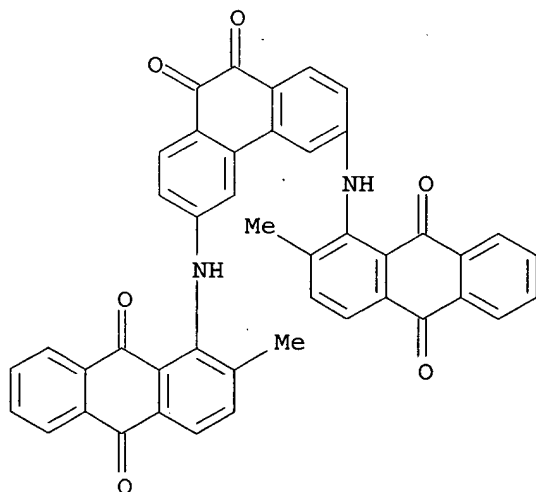


RN 855951-06-3 HCAPLUS

CN Anthraquinone, 1,1'-(9,10-dihydro-9,10-dioxo-3,6-  
phenanthrylenediimino)bis[5-amino- (5CI) (CA INDEX NAME)



RN 855951-13-2 HCAPLUS  
 CN Anthraquinone, 1,1'-(9,10-dihydro-9,10-dioxo-3,6-phenanthrylenediimino)bis[2-methyl- (5CI) (CA INDEX NAME)



L48 ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1953:10779 HCAPLUS  
 DOCUMENT NUMBER: 47:10779  
 ORIGINAL REFERENCE NO.: 47:1933a-i,1934a  
 TITLE: New intermediates and **dyes**. III.  
 Condensation of 4-tert-butylphthalic anhydride with  
 acenaphthene. 6-tert-Butylquinizarin and derived  
 cellulose acetate **dyes**  
 AUTHOR(S): Larner, Brian W.; Peters, Arnold T.  
 CORPORATE SOURCE: Univ. Leeds, UK  
 SOURCE: Journal of the Chemical Society, Abstracts (1952)  
 1368-73  
 CODEN: JCSAAZ; ISSN: 0590-9791  
 DOCUMENT TYPE: Journal



## LANGUAGE:

Unavailable

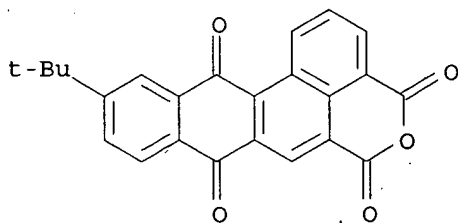
AB cf. C.A. 46, 9540c. PhOH (37 g.), 20 g. 4-tert-BuC<sub>6</sub>H<sub>3</sub>(CO)<sub>2</sub>O (I), and 54 g. ZnCl<sub>2</sub>, heated 2 h. at 120°, raised to 160° in 1 h., and heated 3 h. at 160°, give 18 g. tert-butylphenolphthalein, m. 300-13°, deep red color in concentrated H<sub>2</sub>SO<sub>4</sub>. I (5.1 g.), 5.5 g. m-C<sub>6</sub>H<sub>4</sub>(OH)<sub>2</sub>, and 2 g. ZnCl<sub>2</sub>, heated to 200° (1 h.) and 1 h. at 200°, give 82% tert-butylfluorescein (II), yellow, m. 332-40°. Br (8 g.) was added to a suspension of 4 g. tert-butyl-fluorescein in 20 cc. absolute EtOH, heat developed, and the whole was kept for an hr. There were obtained 1.2 g. orange prisms of tert-butyleosin, m. 314° (decomposition), and 2.7 g. of a solvate (2 mols. EtOH), orange red, m. 248.5-9°. I (10.2 g.) and 7.7 g. acenaphthene (III) in 250 cc. C<sub>6</sub>H<sub>6</sub>, treated with 13.3 g. anhydrous AlCl<sub>3</sub> (temperature below 30°), kept overnight at room temperature, decomposed with dilute HCl, distilled with steam, the product extracted with boiling 10% aqueous Na<sub>2</sub>CO<sub>3</sub>, the alkaline extract acidified, the solid crystallized from AcOH [m. 260° (decomposition), 80%], and then precipitated from cold MeOH with HCl, give 5-(5-tert-butyl-2-carboxybenzoyl)acenaphthene (C.A. numbering) (IV), m. 271-3°; Me ester, pale yellow, m. 139-40°; Et ester, yellow, m. 123-4°. IV (4 g.), 0.4 g. Cu bronze, and 10 cc. quinoline, heated 30 min. at 215-20°, give 5-(m-tert-butylbenzoyl)acenaphthene (V), m. 110-11°; 3.8 g. III, 5 g. m-tert-BuC<sub>6</sub>H<sub>4</sub>COCl, and 5 g. AlCl<sub>3</sub>, 5 h. at room temperature and 30 min. at the b.p., give 41% V. III (7.7 g.) and 10 g. p-tert-BuC<sub>6</sub>H<sub>4</sub>COCl in 50 cc. C<sub>6</sub>H<sub>6</sub>, treated with 10 g. AlCl<sub>3</sub>, kept 3 h. at room temperature, and refluxed 15 min. give 65% of the p-isomer of V, b<sub>6</sub> 280° (oxime, m. 175-7°). III (2 g.) and 6 g. (COCl)<sub>2</sub>, heated at 140°, give 5-acenaphthoic acid, m. 217-18°; with m-tert-BuC<sub>6</sub>H<sub>4</sub>MgBr this yields a product, b<sub>0.7</sub> 185°, m. 170-2°. V with fuming H<sub>2</sub>SO<sub>4</sub> gives only sulfonated products; 7.2 g. V, 24 g. AlCl<sub>3</sub>, and 6 g. NaCl, heated 30 min. at 130° and 30 min. at 140°, give 18% 5,6-(4-tert-butylphthaloyl)acenaphthene (VI), yellow, m. 188-9°. VI (2 g.) in 60 cc. boiling AcOH, treated with 8 g. Na<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>, refluxed 4 h., and extracted with boiling 10% aqueous Na<sub>2</sub>CO<sub>3</sub>, gives 27% 4,5-(4-tert-butylphthaloyl)-1,8-naphthalic anhydride, pale yellow, m. 310°. V (3.6 g.) and 10 g. Na<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in 75 cc. AcOH, refluxed 6 h., give 72% 4-(5-tert-butyl-2-carboxybenzoyl)-1,8-naphthalic anhydride (VII), yellow, m. 238-40°; heating VII with o-C<sub>6</sub>H<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub> in boiling AcOH gives the benziminazole derivative, C<sub>30</sub>H<sub>22</sub>O<sub>4</sub>N<sub>2</sub>, orange, m. 300-2°. VII (2 g.), 2 g. boric anhydride, and 6 cc. fuming H<sub>2</sub>SO<sub>4</sub>, heated 4 h. at 140-60° and extracted with warm 10% aqueous Na<sub>2</sub>CO<sub>3</sub>, give 16% 7-tert-butyl-1,2-benzanthraquinone-3,4'-dicarboxylic anhydride, yellowish green, m. 286°. I (12.8 g.) and 6.4 g. p-ClC<sub>6</sub>H<sub>4</sub>OH in 30 cc. CCl<sub>4</sub>, treated with 13.3 g. AlCl<sub>3</sub> and heated 3 h. on the steam bath, give 6(or 7)-tert-butyl-1-chloro-4-hydroxyanthraquinone (VIII), greenish yellow needles, m. 150-2°. H<sub>3</sub>BO<sub>3</sub> (6 g.) in 98% H<sub>2</sub>SO<sub>4</sub> at 50°, treated alternatively in portions (1 h.) with 15.3 g. I and 6.4 g. p-ClC<sub>6</sub>H<sub>4</sub>OH, the temperature raised to 160° in 2 h., heated 3 h. at 160°, raised to 210° in 1 h., and heated 2 h. at 210°, cooled to 100°, treated with 20 cc. 98% H<sub>2</sub>SO<sub>4</sub> and 33 cc. H<sub>2</sub>O, poured onto ice, the precipitate boiled 10 min. with 300 cc. H<sub>2</sub>O, the product extracted with boiling 2% aqueous NaOH, acidified, and crystallized from PhCl, give 2.2 g. 6-tert-butylquinizarin (IX), bright red, m. 169-71°; 0.8 g. VIII, added to 6 g. H<sub>3</sub>BO<sub>3</sub> in 8 cc. 98% H<sub>2</sub>SO<sub>4</sub> and heated 6 h. at 190°, gives 80% IX. I (12.8 g.) and 5.5 g. p-C<sub>6</sub>H<sub>4</sub>(OH)<sub>2</sub> with AlCl<sub>3</sub> in CCl<sub>4</sub> give 2.1 g. IX; in the 2nd method, the use of p-C<sub>6</sub>H<sub>4</sub>(OH)<sub>2</sub> gives 1.5 g. IX. I (26 g.) and 11 g. p-C<sub>6</sub>H<sub>4</sub>(OH)<sub>2</sub>, gradually added to 10 g. NaCl

and 50 g.  $\text{AlCl}_3$  at  $130^\circ$  and heated 5 h. at  $140^\circ$ , give 6.5 g. IX. IX (2 g.), 2 g.  $\text{Na}_2\text{S}_2\text{O}_4$ , and 12 cc.  $\text{NH}_4\text{OH}$  (d. 0.88), heated 7 h. at  $145-50^\circ$ , give 90% 1,4-diamino-6-tert-butylantraquinone, violet with Cu luster, m.  $223-4^\circ$ ; **dyes** cellulose acetate rayon a deep magenta shade; the rayon, milled with Tannadol and  $\text{H}_2\text{O}$  and dyed at  $65-85^\circ$ , was redder and duller than that dyed with 1,4-diaminoanthraquinone but was slightly more resistant to gas-fume fading. IX (1 g.), 1 g.  $\text{Na}_2\text{S}_2\text{O}_4$ , and 6 cc. 33% aqueous  $\text{MeNH}_2$ , 7 h. at  $145-50^\circ$ , give 88% 6-tert-butyl-1,4-bis(methylamino)anthraquinone, dark blue with bronze luster, m.  $142^\circ$ ; the dyeings of rayon were greener and duller than those shown by the analogous 1,4-bis-(methylamino) derivative and possessed similar gas-fume fading-fastness

IT 857536-88-0, Benz[a]anthracene-4,5-dicarboxylic anhydride, 10-tert-butyl-7,12-dihydro-7,12-dioxo- (preparation of)

RN 857536-88-0 HCAPLUS

CN Benz[a]anthracene-4,5-dicarboxylic anhydride, 10-tert-butyl-7,12-dihydro-7,12-dioxo- (5CI) (CA INDEX NAME)



L48 ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1944:22726 HCAPLUS

DOCUMENT NUMBER: 38:22726

ORIGINAL REFERENCE NO.: 38:3281h-i,3282a-e

TITLE: 6,7,6',7'-Diphthaloylisooxindigotin, its derivatives and its isomerization. I

AUTHOR(S): Marschalk, Ch.

SOURCE: Bull. soc. chim. (1942), 9, 826-32

DOCUMENT TYPE: Journal

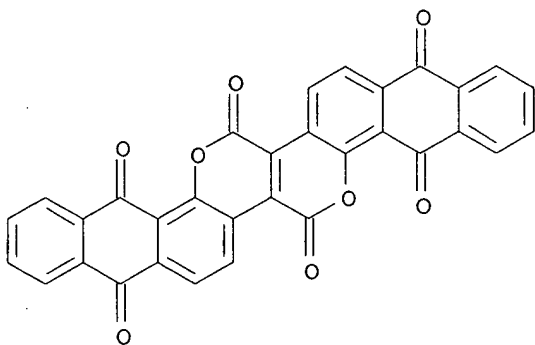
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB 6,7,6',7'-Diphthaloylisooxindigotin (I, R =  $-\text{CO.C}_6\text{H}_4.\text{CO}-$ ) was prepared by heating 1-hydroxy-2-anthraquinoneacetic acid (II) with  $\text{SOCl}_2$  in  $\text{PhNO}_2$  or xylene at  $100^\circ$ , by heating 6,7-phthaloyl-2-coumaranone (III) in the same manner with  $\text{S}_2\text{Cl}_2$  in  $\text{PhNO}_2$  or xylene at  $130^\circ$  or with  $\text{FeCl}_3$  or  $\text{CrO}_3$  in  $\text{AcOH}$  or with Br in boiling  $\text{PhNO}_2$ , and by condensing 6,7-phthaloyl-2,3-coumarandione 3-p-dimethylaminoanil with 6,7-phthaloyl-2-coumaranone in boiling  $\text{Ac}_2\text{O}$ . It forms orange-red rhombohedrons from  $\text{PhNO}_2$ , m.  $448^\circ$  (Au block).  $\text{S}_2\text{Cl}_2$  and  $\text{FeCl}_3$  have no effect on II. It can be assumed with certainty that III is an intermediate product in the formation of I from II. Heating I on the  $\text{H}_2\text{O}$  bath with  $\text{H}_2\text{SO}_4$  yielded 4,5,4',5'-diphthaloyl-3,4,7,8-dibenzonaphthyrone (IV), yellow crystals from  $\text{PhNO}_2$ , m.  $491^\circ$ . IV was also prepared by heating with  $\text{H}_2\text{SO}_4$  in the same manner the acid (V) formed by alkaline hydrolysis of I and IV. Short boiling of V with  $\text{Ac}_2\text{O}$  or  $\text{SOCl}_2$  in  $\text{PhNO}_2$  gave a yellow-orange **dye**. V was probably a mixture of 2 acids. Expts. on converting V into I always yielded an appreciable amount of IV, indicating IV to be the stabler compound According to Chovin (Bulletin society chim. 8,645(1941); cf. C. A. 37, 2737.1) the isooxindigotin derivs. are

yellow and the naphthyrones orange-red. M.'s exptl. results contradict these conceptions. The color of I agrees with its assigned constitution because the true indigoid condensation product of III and acenaphthenequinone is orange-red just as is bis-(acenaphthene) indigotin, itself.

IT 854389-14-3, 6,16-Dioxabenzob[naphtho[2,3-m]picene-5,7,10,15,17,20-hexone  
(preparation of)  
RN 854389-14-3 HCAPLUS  
CN 6,16-Dioxabenzob[naphtho[2,3-m]picene-5,7,10,15,17,20-hexone (4CI) (CA INDEX NAME)



L48 ANSWER 19 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1943:25227 HCAPLUS

DOCUMENT NUMBER: 37:25227

ORIGINAL REFERENCE NO.: 37:4065i,4066a-i,4067a-d

TITLE: Derivatives of 3',2-acenaphthoylbenzoic acid

AUTHOR(S): Peters, A. T.; Rowe, F. M.

SOURCE: Journal of the Society of Dyers and Colourists (1943), 59, 52-4

CODEN: JSDCAA; ISSN: 0037-9859

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

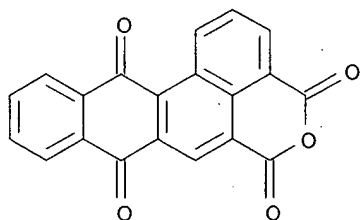
AB Attempts to prepare condensation products from acenaphthenequinone and phthalic anhydride (I) as intermediates of vat dyes failed. But when 50 g. acenaphthene and 52 g. I in 200 cc. C<sub>6</sub>H<sub>6</sub> are stirred with 73 g. AlCl<sub>3</sub> at room temperature for 4 hrs., a resinous product is obtained which, after decantation of the C<sub>6</sub>H<sub>6</sub>, is treated with 50 cc. concentrated HCl in 200 cc. H<sub>2</sub>O. Extraction of the residue with 10% Na<sub>2</sub>CO<sub>3</sub> at 60° and acidification of the aqueous extract give 89.7% 3',2-acenaphthoylbenzoic acid (II), m. 199-200°. When 30 g. II is heated with a mixture of 50 g. AlCl<sub>3</sub> and 40 g. NaCl at 134-5° within 0.5 hr. and kept at this temperature for 3 hrs., decomposition of the reaction mixture with HCl and extraction of the

residue with 10% Na<sub>2</sub>CO<sub>3</sub> leaves 26.6% 3,4-phthaloylacenaphthene (III), m. 194-5° after crystallization from AcOH and EtOH. From the Na<sub>2</sub>CO<sub>3</sub> solution 12 g. unchanged II is recovered. III dissolves in concentrated H<sub>2</sub>SO<sub>4</sub> with an orange color and strong green fluorescence. The mono-p-nitrophenylhydrazone of III m. 255-6° and dissolves in concentrated H<sub>2</sub>SO<sub>4</sub> with a deep reddish brown color without fluorescence. The mono-2,6-dichloro-4-nitrophenylhydrazone m. 248-9° (decomposition). Mild oxidation of III by heating it with Na<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in AcOH for 3 min. gives orange crystals (IV), m. 330-50° (decomposition) after sintering at

258-60°. IV is either a double compound or a mixture of III and 4,5-phthaloylnaphthalic anhydride (V). When IV is extracted with boiling alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> and the residue crystallized, III is obtained; extraction of IV with pyridine gives V. On more drastic oxidation of III by refluxing it for 20 min. with Na<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in AcOH, 84.4% V is obtained. V is soluble in warm NaOH and on addition of Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> gives a magenta color changing to orange-brown. It is soluble in concentrated H<sub>2</sub>SO<sub>4</sub> with a deep orange color. On fusion with m-C<sub>6</sub>H<sub>4</sub>(OH)<sub>2</sub> V gives a product soluble in dilute NaOH with a strong green fluorescence but no crystalline compound can be isolated. The di-p-nitrophenylhydrazone of V, deep orange-red prisms, m. 287-8° (decomposition); bis (2,6-dichloro-4-nitrophenylhydrazone), orange prisms, m. about 200°. V refluxed with concentrated NH<sub>4</sub>OH for 3 hrs. gives 84% imide as pale yellow needles, decomposing gradually above 390°. It does not give a hydrazone. With 33% aqueous NH<sub>2</sub>Me, V gives the N-methylimide, m. 315-16°. When V is fused with p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>, 4,5-phthaloyl-4'-nitronaphthanil, colorless needles, m. about 400°, is obtained. When 1 mol. V and 1.1 mols. o-C<sub>6</sub>H<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub> are refluxed in AcOH for 10 min., 86.3% 9'-keto-3',4'-phthaloyl-8'-azaphenalino(7',8',2,3)-ψ-indole (VI), orange needles, m. 380°, is formed. VI is insol. in NaOH but soluble in concentrated H<sub>2</sub>SO<sub>4</sub> with orange-red color. With alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> a deep reddish violet vat is formed which dyes cotton golden-yellow. As ring closure proceeds more easily with o-carboxybenzyl derivs., II is reduced in alkaline alc. solution with Zn dust, giving a mixture of 3',2-acenaphthylmethylbenzoic acid (VII) and its lactone (VIII). It is separated by extraction with Na<sub>2</sub>CO<sub>3</sub> solution and the insol. VIII recrystd. from CHCl<sub>3</sub> in a yield of 27.5%. VIII m. 201-2° and dissolves in concentrated H<sub>2</sub>SO<sub>4</sub> with a deep reddish violet color which soon changes to olive-green. Acidification of the Na<sub>2</sub>CO<sub>3</sub> extract gives 57.7% VII, m. 211-12°. VII dissolves in concentrated H<sub>2</sub>SO<sub>4</sub> with a yellowish brown color. VII is also obtained in 81.8% yield by refluxing 18 g. II with 500 cc. 2 N NaOH, 33 g. Zn dust and 75 cc. of a solution of equal vols. 2 N NH<sub>4</sub>OH and 2 N CuSO<sub>4</sub> for 50 hrs. (cf. Scholl and Neovius, C. A. 5, 2830). When 10 g. 4-o-carboxybenzoylnaphthalic anhydride (IX), m. 236°, is heated with 12 g. H<sub>3</sub>BO<sub>3</sub> and 30 cc. 20% fuming H<sub>2</sub>SO<sub>4</sub> within 2 hrs. to 150° and kept there for 3 hrs., addition of H<sub>2</sub>O causes a precipitate which, after extraction with warm Na<sub>2</sub>CO<sub>3</sub> solution and recrystn. from PhNO<sub>2</sub>, gives 64.2% 3,4-phthaloylnaphthalic anhydride (X), greenish yellow prismatic needles, m. 315°. When IX is heated with concentrated H<sub>2</sub>SO<sub>4</sub> for 5 hrs. at 180-5°, 63.1% X is obtained. X dissolves in cold alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> solution with a deep brownish red color. Mono-p-nitrophenylhydrazone of X m. 350-3° (decomposition); the imide (XI), m. 360° (decomposition) after darkening at 345°, is obtained in 80% yield by heating X with NH<sub>4</sub>OH. XI dissolves in alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> with a deep bluish green color. XI is also formed in 73.8% yield when 4-o-carboxybenzoyl-1,8-naphthalimide (XII), m. 296-7°, is heated with 20% fuming H<sub>2</sub>SO<sub>4</sub> at 160° for 3 hrs. In an attempt to effect ring closure according to Heidenreich (C. A. 25, 3668) by heating XII with concentrated H<sub>2</sub>SO<sub>4</sub> at 185-230°, X is formed with elimination of NH<sub>3</sub>. The N-methylimide (XIII), obtained in 81.8% yield by heating X with 33% NH<sub>2</sub>Me, m. 276-7°. 4-o-Carboxybenzoyl-1,8-naphthal-N-methylimide, formed in 80.4% yield from IX, m. 238-9° and on crystallization from concentrated H<sub>2</sub>SO<sub>4</sub> gives 72% XIII. 3,4-Phthaloyl-4'-nitronaphthalanil, yellow needles, m. above 380°. X and o-C<sub>6</sub>H<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub> give 81.7% 9'-keto-4',5'(or 2',3')-phthaloyl-8'-azaphenalino (7',8',2,3)-ψ-indole (XIV) m. 320-5°. XIV dissolves in concentrated H<sub>2</sub>SO<sub>4</sub> with a brownish yellow color; its olive-green

alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> vat **dyes** cotton orange. IX and o-C<sub>6</sub>H<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub> give 91.1% 9'-keto-4' (or 3')-o-carboxybenzoyl-8'-azaphenalino(7',8',2,3)-ψ'-indole (XV), bright yellow needles, m. 285-7°. XV is soluble in alkali. Attempted ring closure with 20% fuming H<sub>2</sub>SO<sub>4</sub> with or without H<sub>3</sub>BO<sub>3</sub> at 150-60° or with AlCl<sub>3</sub> at 190° gives only a trace of XIV.

IT 22245-71-2, Naphthalic anhydride, 3,4-phthaloyl-  
(preparation of)  
RN 22245-71-2 HCAPLUS  
CN 4H,6H-Anthra[3,2,1-de][2]benzopyran-4,6,8,13-tetrone (9CI) (CA INDEX NAME)



L48 ANSWER 20 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1925:21696 HCAPLUS

DOCUMENT NUMBER: 19:21696

ORIGINAL REFERENCE NO.: 19:2822e-g

TITLE: Fungus dyestuffs. II. The **dye** of the blood-red "Hautkopf" (*Dermocybe sanguinea* Wulf.)

AUTHOR(S): Kogl, Fritz; Postowsky, J. J.

SOURCE: Ann. (1925), 444, 1-7

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

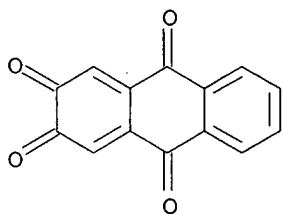
AB cf. C. A. 19, 639. The fungus, *Dermocybe sanguinea* Wolf., was dried, extracted with EtOH, the residue of the extract treated with 3% NH<sub>4</sub>OH and, after

filtering, the **dye** precipitated by acid. Adding 10 vols. H<sub>2</sub>O to the C<sub>5</sub>H<sub>5</sub>N solution ppts. emodin (3% yield of the dry powder); dilute HCl ppts. from the filtrate a new **dye**, dermocybin, C<sub>16</sub>H<sub>12</sub>O<sub>7</sub> (I), red needles, m: 228-9°, soluble in concentrated H<sub>2</sub>SO<sub>4</sub> with a deep violet, in alkali with a red-violet color; it **dyes** Cr-mordanted wool a violet-red. The spectra are given for concentrated and dilute H<sub>2</sub>SO<sub>4</sub> and 0.1 N NaOH. Tetra-Ac derivative, yellow, m. 182°. Concentrated H<sub>2</sub>SO<sub>4</sub> splits off 1 Me group, giving a pentahydroxy-β-methylantraquinone, red, m. 289°; the solns. in concentrated H<sub>2</sub>SO<sub>4</sub> and alkali have the same colors as I and **dye** wool the same color. The spectra in concentrated H<sub>2</sub>SO<sub>4</sub> and in Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> solution are given. Distillation with Zn dust gives β-methylanthrane. I is therefore a pentahydroxymethoxy-β-methylantraquinone.

IT 5599-74-6, 2,3,9,10-Anthracenetetrone  
(preparation of)

RN 5599-74-6 HCAPLUS

CN 2,3,9,10-Anthracenetetrone (7CI, 8CI, 9CI) (CA INDEX NAME)



L48 ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1922:10119 HCAPLUS

DOCUMENT NUMBER: 16:10119

ORIGINAL REFERENCE NO.: 16:1767h-i,1768a-i,1769a

TITLE: Action of bromine on quinizarin and alizarin

AUTHOR(S): Dimroth, Otto; Schutze, Ernst; Heinze, Fritz

SOURCE: Ber. (1921), 54B, 3035-50

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C. A. 14, 3073. This study of the action of Br on simple hydroxyanthraquinones was undertaken to clear up the individual stages of its action on carminic and kermesic acids and thus to determine the structures of these 2 **dyes**. Quinizarin (A) dissolves at 0° in liquid Br and in a few min. the solution solidifies with deposition of red crystals of a very loose Br addition product which at once again loses its Br in the air; on standing several days, it redissolves, Liebermann's hexabromide being slowly formed (Ber. 33, 1658(1900)). A is unchanged by Br water at room temperature, even after shaking for a day, but by Br in KBr is rapidly oxidized to quinizarinquinone (B). B is a much stronger oxidizing agent than benzoquinone or most other quinones, oxidizing leucomalachite green in AcOH instantly to the **dye** and not only HI to I but even HBr to Br; there exists the equilibrium  $A + Br \rightleftharpoons B + HBr$  and in order to effect the oxidation  $A \rightarrow B$ , the Br must be present in excess of a certain minimum concentration: this minimum concentration is not attained in

Br water

but is in Br-KBr solution, hence the results reported above. With Br water in the presence of liquid Br, A gives a compound (C), isomeric with L.'s dibromoquinizarin (D), which has quinone properties, liberating I from HI and oxidizing leucomalachite green; with  $Ac_2O-H_2SO_4$  it gives the diacetate of D; it liberates 4 atoms I from HI, with formation of A. C must therefore be quinizarin-quinone dibromide; it can also be obtained from B and Br. With  $SO_2$ , C gives bromoquinizarin (E); apparently  $SO_2$  first attacks the quinone O, forming quinizarin dibromide which at once loses HBr and yields E, while HI on the other hand first removes the halogen and then reduces the resulting B to A. C easily loses HBr, very slowly on standing, quickly on boiling with AcOH or  $H_2O$ ; the resulting bromoquinizarinquinone, under the conditions of the HBr cleavage, is at once reduced to E and the HBr oxidized to Br. The complete reaction may therefore be represented by the scheme:  $A \rightarrow \text{addition compound} \rightarrow B \rightarrow C \rightarrow E$ . That bromination by the usual methods (e. g., that of Liebermann in boiling AcOH), in which the final product, E, seems to result from a simple substitution reaction, follows the same complicated course is indicated by the following facts: When A is shaken some hrs. at room temperature with Br in AcOH the characteristic needles of B sep. and again disappear; B rapidly and smoothly adds Br in boiling AcOH, a reaction not impeded by the presence of HBr; C in boiling AcOH decomps. into E and if HBr is present the HBr is oxidized to Br and the yield of E

is quant. Alizarin (F) with Br water, with Br-KBr and with Br water in the presence of liquid Br yields in all 3 cases the same compound, red crystals so unstable that their composition could not be determined with certainty

but which with SO<sub>2</sub> give 3-bromoalizarin (G) and about 1 mol. HBr and are doubtless alizarinquinone dibromide; H<sub>2</sub>O quickly changes them into 3-bromoalizarinquinone (H), reduced by SO<sub>2</sub> or HI to G which with Br or Pb(OAc)<sub>4</sub> regenerates H. With Br in MeOH, A gives quinizarinquinone methoxybromide (I), C<sub>6</sub>H<sub>4</sub>(CO)<sub>2</sub>, which liberates 4 atoms of I from HI, with regeneration of A, and is rearranged by Ac<sub>2</sub>O and a trace of H<sub>2</sub>SO<sub>4</sub> into the diacetate (J) of 3-bromopurpurin 2-methyl ether (K); SO<sub>2</sub> also reduced I to A. F similarly yields alizarinquinone methoxybromide (L), reduced by HI or SO<sub>2</sub> to G and rearranged by Ac<sub>2</sub>O-H<sub>2</sub>SO<sub>4</sub> into diacetyl-3-bromopurpurin 4-methyl ether (M). Bromination of F in MeOH with gentle warming gives 3,4-dibromoalizarin (N), oxidized by KMnO<sub>4</sub> to phthalic acid. Bromination of F in EtOH proceeds as in MeOH. C seps. from CHCl<sub>3</sub>-ligroin in fine, faintly pink needles, m. 210-5° (decomposition). E crystallizes from AcOH, C<sub>5</sub>H<sub>5</sub>N or (CHCl<sub>3</sub>)<sub>2</sub> in red needles, m. 228-30°, forms in dilute KOH a blue solution with absorption bands at 560-70 and 595-610 μμ, in concentrated H<sub>2</sub>SO<sub>4</sub> a light red solution without perceptible fluorescence and

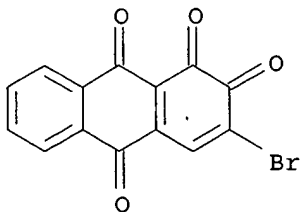
the

same bands (510-20 and 545-60 μμ) as A; diacetate, light yellow needles from AcOH, m. 216-8°. D, crystals from (CHCl<sub>3</sub>)<sub>2</sub>, m. 252-3°, forms in dilute KOH a blue solution with bands at 565-75 and 600-10 μμ, in H<sub>2</sub>SO<sub>4</sub> a violet solution with bands at 515-20 and 550-60 μμ; diacetate, pale yellow needles, m. 270-1°. I, stout yellow crystals from C<sub>6</sub>H<sub>6</sub>-ligroin, becomes superficially brown in the light, m. 90°. J, light yellow crystals from C<sub>6</sub>H<sub>6</sub>, m. 145°, hydrolyzed by boiling concentrated H<sub>2</sub>SO<sub>4</sub> to K, red needles from PhNO<sub>2</sub>, C<sub>5</sub>H<sub>5</sub>N or AcOH, m. 260°, forms in dilute KOH a red solution with bands at 500-10 and 535-45 μμ, in H<sub>2</sub>SO<sub>4</sub> a red solution with bands at 480-90 and 515-25 μμ, addition of H<sub>3</sub>BO<sub>3</sub> making the solution violet with bands at 500-10 and 535-45 μμ. K is also obtained from purpurin 2-Me ether and Br in AcOH under a reflux. H, yellow needles from CHCl<sub>3</sub>-ligroin, decomp. on long standing or in the light. L, yellow lancet-shaped needles from CHCl<sub>3</sub>-petr. ether, decomp. about 200°, sinters and m. around 230°. N, yellow needles from AcOH, m. 251-2°, soluble in alkali with a redder tinge than F, in H<sub>2</sub>SO<sub>4</sub> with K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> color which does not change with H<sub>3</sub>BO<sub>3</sub>; diacetate, light yellow needles from AcOH, m. 199-200°. N with Br-KBr gives dark crystals changed by H<sub>2</sub>O into the egg-yellow 3,4-dibromoalizarinquinone. Alizarinquinone ethoxybromide, yellow tablets from CHCl<sub>3</sub>-petr. ether, sinters 180°, m. about 205° (decomposition).

IT 18378-49-9, 1,2,9,10-Anthracenetetrone, 3-bromo-  
56018-71-4, 1,2,9,10-Anthracenetetrone, 3,4-dibromo-  
(preparation of)

RN 18378-49-9 HCAPLUS

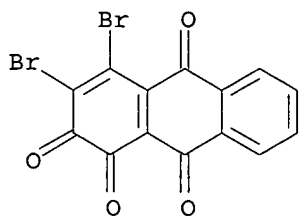
CN 1,2,9,10-Anthracenetetrone, 3-bromo- (8CI) (CA INDEX NAME)



Powers 09\_927685

RN 56018-71-4 HCAPLUS

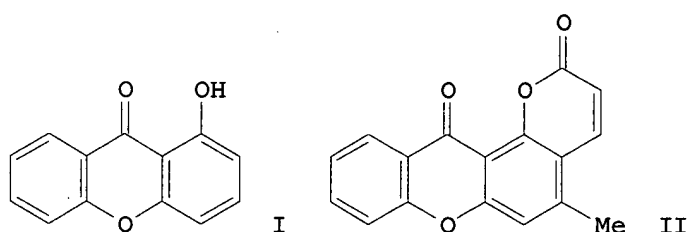
CN 1,2,9,10-Anthracenetetrone, 3,4-dibromo- (9CI) (CA INDEX NAME)



=>



AN 1983:575540 CAPLUS  
DN 99:175540  
TI Studies in synthesis of xanthone derivatives: Part III. A new one-step synthesis of xanthenes  
AU Patolia, Ravji J.; Trivedi, K. N.  
CS Fac. Sci., M. S. Univ. Baroda, Baroda, 390 002, India  
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(5), 444-7  
CODEN: IJSBDB; ISSN: 0376-4699  
DT Journal  
LA English  
OS CASREACT 99:175540  
GI



AB Et salicylate condenses with different phenols in refluxing Ph<sub>2</sub>O to give various xanthenes, e.g., I, in good yields. With resorcinol, hydroquinone, catechol, and 3,4-xyleneol, the corresponding Ph salicylate derivs. are also obtained. Condensation with hydroxycoumarins gives pyranoxanthenes, e.g., II, which can not be prepared by the Pechmann condensation of hydroxyxanthenes. The structures of the intermediates and final products are established by spectral data (IR, H and <sup>13</sup>C NMR).